Supplemental Material to Anisotropic swim stress in active matter with nematic order

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I. GENERALIZED TAYLOR DISPERSION THEORY

In this section we follow the Generalized Taylor Dispersion Theory (GTDT) by Frankel and Brenner [1] to derive the anisotropic swim diffusivity $\boldsymbol{D}^{swim}$ and the ideal gas swim stress $\boldsymbol{\sigma}^{swim} = -n\zeta\boldsymbol{D}^{swim}$. Similar methods have also been used by Zia and Brady [2] and by Takatori and Brady [3]. In the $\boldsymbol{B}$-field theory by Frankel and Brenner [1], $\boldsymbol{q}$ is a local degree of freedom. For the swimmers considered here, $\boldsymbol{q}$ is the orientation vector of each swimmer. The steady state distribution, $P_0^\infty(\boldsymbol{q})$, is analytically solvable from the balance of rotational flux $\boldsymbol{j}_R$:

$$\boldsymbol{j}_R = \boldsymbol{\omega}(\boldsymbol{q};\hat{\boldsymbol{H}})P - \boldsymbol{D}_R\cdot\nabla_R P, \quad \nabla_R\cdot\boldsymbol{j}_R = 0, \tag{1}$$

where $\hat{\boldsymbol{H}}$ is the unit vector in the direction of the orienting field, $\boldsymbol{\omega}(\boldsymbol{q};\hat{\boldsymbol{H}})$ is the angular velocity. $\boldsymbol{D}_R$ is the *intrinsic* rotational diffusivity, which could be an anisotropic tensor.

The orientation-average velocity is defined as:

$$\langle\boldsymbol{U}\rangle = \int_{\boldsymbol{q}} P_0^\infty(\boldsymbol{q})\boldsymbol{U}(\boldsymbol{q})d\boldsymbol{q}. \tag{2}$$

By decomposing $\Delta\boldsymbol{U}(\boldsymbol{q}) = \boldsymbol{U}(\boldsymbol{q}) - \langle\boldsymbol{U}\rangle$, the effective diffusivity is given by

$$\boldsymbol{D}^{swim} = \int_{\boldsymbol{q}} P_0^\infty(\boldsymbol{q})\boldsymbol{B}(\boldsymbol{q})\Delta\boldsymbol{U}(\boldsymbol{q})d\boldsymbol{q}, \tag{3}$$

where the $\boldsymbol{B}$ field is the solution to

$$\nabla_{\boldsymbol{q}}\cdot[\boldsymbol{\omega}P_0^\infty\boldsymbol{B} - \boldsymbol{D}_R\cdot\nabla_{\boldsymbol{q}}(P_0^\infty\boldsymbol{B})] = \Delta\boldsymbol{U}P_0^\infty, \tag{4}$$

$$\int_{\boldsymbol{q}} P_0^\infty\boldsymbol{B}d\boldsymbol{q} = 0, \tag{5}$$

with appropriate BCs in $\boldsymbol{q}$ space. Here $\boldsymbol{\omega}$ and $\boldsymbol{D}_R$ are angular velocity and (intrinsic) rotational diffusivity in $\boldsymbol{q}$ space, respectively. Physically, $\boldsymbol{B}(\boldsymbol{q})$ represents the fluctuation of $\boldsymbol{q}$ as a function of $\boldsymbol{q}$. This fluctuation in the orientational space propagates to the translational motion physical space through the disturbance velocity $\Delta\boldsymbol{U}(\boldsymbol{q})$.

For an orientational potential energy $V(\boldsymbol{q})$, the torque and angular velocity are:

$$\boldsymbol{L} = -\nabla_R V, \qquad \boldsymbol{\omega} = \frac{1}{\zeta_R}\boldsymbol{L}, \tag{6}$$

where we assumed the isotropic orientational drag ζ_R. The angular velocity is interpreted as:

$$\dot{\boldsymbol{q}} = -\boldsymbol{q}\times\boldsymbol{\omega}\,. \tag{7}$$

In this work we considered a special case where the potential energy $V(\boldsymbol{q}) = -\epsilon(\boldsymbol{q}\cdot\hat{\boldsymbol{H}})^2$ is given by the bistable form in the main text. The direction of $V(\boldsymbol{q})$ is denoted by $\hat{\boldsymbol{H}}$. The parameter $\chi_R = \epsilon/k_BT$ sets the nondimensional strength of the potential.

II. CASE 1. SWIMMERS IN A 2D LAYER: IN-PLANE ROTATION.

The rotational space for in-plane rotation is represented by a single angle $\theta\in[-\pi,\pi)$. Let $\cos\theta = \boldsymbol{q}\cdot\hat{\boldsymbol{H}}$. At steady state, the equilibrium orientation distribution is:

$$P_0^\infty(\theta) = \frac{1}{2\pi I_0(\chi_R/2)}e^{\frac{1}{2}\chi_R\cos(2\theta)}, \tag{8}$$

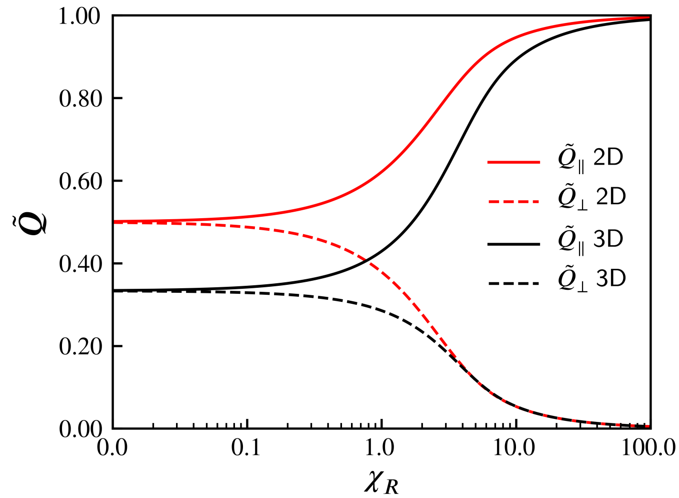

FIG. 1. The nematic order parameter $\tilde{\boldsymbol{Q}} = \langle \boldsymbol{qq} \rangle$ as a function of field strength $\chi_R = \epsilon/k_B T$.

where I_0 is the Bessel function. $P_0^\infty(\theta)$ is normalized so that $\int_{-\pi}^{\pi} P_0^\infty d\theta = 1$. The nematic order parameter $\tilde{\boldsymbol{Q}}$ is:

$$\langle \boldsymbol{q}_\parallel \boldsymbol{q}_\parallel \rangle = \frac{1}{2}\left(\frac{I_1(\chi_R/2)}{I_0(\chi_R/2)} + 1\right), \tag{9a}$$

$$\langle \boldsymbol{q}_\perp \boldsymbol{q}_\perp \rangle = \frac{1}{2}\left(-\frac{I_1(\chi_R/2)}{I_0(\chi_R/2)} + 1\right). \tag{9b}$$

Here we also have $\mathrm{Tr}\,\tilde{\boldsymbol{Q}} = 1$, as required by the definition of $\tilde{\boldsymbol{Q}}$. The zero-traced nematic order parameter $\boldsymbol{Q}$ is defined as $\boldsymbol{Q} = \tilde{\boldsymbol{Q}} - \frac{1}{2}\boldsymbol{I}$ for the 2D case. The order parameter $\tilde{\boldsymbol{Q}}$ is shown in Fig. 1.

GTDT gives the $\boldsymbol{B}$ field in the two directions parallel and perpendicular to $\hat{\boldsymbol{H}}$:

$$B_\parallel(\theta) = -\int_0^\theta \frac{\sqrt{\pi} e^{\chi_R \sin^2\kappa} \mathrm{Erf}\left(\sqrt{\chi_R}\sin\kappa\right)}{2\sqrt{\chi_R}} d\kappa, \tag{10a}$$

$$B_\perp(\theta) = \int_0^\theta \frac{F_D\left(\sqrt{\chi_R}\cos\kappa\right)}{\sqrt{\chi_R}} d\kappa, \tag{10b}$$

where $F_D(z)$ is the Dawson-F integral function:

$$F_D(z) = e^{-z^2} \int_0^z e^{y^2} dy. \tag{11}$$

The swim diffusivity comes from the orientational fluctuation $\boldsymbol{B}$:

$$\hat{D}_\parallel^{swim} = \frac{D_\parallel^{swim}}{U_0^2/2} = -2\int_{-\pi}^{\pi}\int_0^\theta \frac{\sqrt{\pi} e^{\chi_R \sin^2\kappa} \mathrm{Erf}\left(\sqrt{\chi_R}\sin\kappa\right)}{2\sqrt{\chi_R}} d\kappa P_0^\infty(\theta)\cos\theta d\theta, \tag{12a}$$

$$\hat{D}_\perp^{swim} = \frac{D_\perp^{swim}}{U_0^2/2} = 2\int_{-\pi}^{\pi}\int_0^\theta \frac{F\left(\sqrt{\chi_R}\cos\kappa\right)}{\sqrt{\chi_R}} d\kappa P_0^\infty(\theta)\sin\theta d\theta, \tag{12b}$$

which are shown in the maintext.

The swim stress follows

$$\hat{\sigma}_\parallel^{swim} = \frac{\sigma_\parallel}{-n\zeta U_0^2/2} = \hat{D}_\parallel^{swim}, \tag{13}$$

$$\hat{\sigma}_\perp^{swim} = \frac{\sigma_\perp}{-n\zeta U_0^2/2} = \hat{D}_\perp^{swim}; \tag{14}$$

for 2D in-plane rotations the isotropic swim pressure is $n\zeta U_0^2/2$, instead of $n\zeta U_0^2/6$.

A. The weak field limit $\chi_R \to 0$.

By direct expansion of (12):

$$\hat{\sigma}_{\parallel}^{swim} \approx 1 + \frac{3\chi_R}{4} + O(\chi_R^2), \tag{15a}$$

$$\hat{\sigma}_{\perp}^{swim} \approx 1 - \frac{3\chi_R}{4} + O(\chi_R^2). \tag{15b}$$

B. The strong field limit $\chi_R \to \infty$.

In this case Kramers' escape rate theory can be directly used since the orientation is a 1D space for θ. For the potential $V(\theta)$, the escape rate out of its minimum is

$$\begin{aligned} r_K &= \frac{1}{2\pi}\sqrt{V''(\theta_{min})\,|V''(\theta_{max})|}e^{-\frac{V(\theta_{max})-V(\theta_{min})}{\zeta D}} \\ &= \frac{\chi_R D_R}{\pi}e^{-\chi_R}, \end{aligned} \tag{16}$$

where $V(\theta_{min})$ and $V(\theta_{max})$ are minimum and maximum of the potential V, respectively. The parallel swim diffusivity $D_{\parallel}^{swim}$ is the result of the 1D random walk in the direction of $\hat{\boldsymbol{H}}$, and

$$\hat{\sigma}_{\parallel}^{swim} = \frac{D_{\parallel}^{swim}}{U_0^2\tau_R/2} \to \frac{\pi}{2}\frac{e^{\chi_R}}{\chi_R}. \tag{17}$$

The limiting transverse diffusivity $D_{\perp}^{swim}$ results from a 'boundary layer' around the equilibrium position $\boldsymbol{q}\cdot\hat{\boldsymbol{H}} = 0$, since at the strong field limit $\theta \approx 0$ (or π) is almost always true. For 2D rotation, it can be directly calculated from the integral with the 'boundary layer' approximation: $\theta \approx \sin\theta,\ \cos\theta \approx 1 - \theta^2/2$. The integrals in (12) are explicitly integrable with these approximations, and:

$$\frac{D_{\perp}^{swim}}{U_0^2\tau_R/2} \approx 8\int_0^{\frac{\pi}{2}} \frac{e^{\frac{1}{2}\chi_R\cos(2\theta)}\sin^2\theta}{4\pi\chi_R I_0\left(\frac{\chi_R}{2}\right)}\,d\theta = \frac{1 - \frac{I_1\left(\frac{\chi_R}{2}\right)}{I_0\left(\frac{\chi_R}{2}\right)}}{2\chi_R} \to \frac{1}{2\chi_R^2}, \tag{18}$$

Therefore:

$$\hat{\sigma}_{\perp}^{swim} = \frac{D_{\perp}^{swim}}{U_0^2\tau_R/2} \to \frac{1}{2\chi_R^2}. \tag{19}$$

The asymptotics in the strong and weak limits are also shown in the main text.

III. CASE 2. SWIMMERS IN 3D SPACE.

In this case the rotation is mathematically challenging to describe. In this work we follow the convention of Brenner and Condiff [4] by defining a nabla operator in orientation space ∇_R. The evolution of a spherical ABP with orientation $\boldsymbol{q}$ by torque and Brownian motion can be described in a spherical coordinate system $(0 < \theta < \pi, 0 < \phi < 2\pi)$:

$$\boldsymbol{q} = \sin\theta\cos\phi\boldsymbol{e}_x + \sin\theta\sin\phi\boldsymbol{e}_y + \cos\theta\boldsymbol{e}_z \tag{20}$$

The rotational gradient operator $\nabla_R = \boldsymbol{q} \times \dfrac{\partial}{\partial \boldsymbol{q}}$. Here we have:

$$\frac{\partial f(\theta,\phi)}{\partial \boldsymbol{q}} = \boldsymbol{e}_\theta\frac{\partial f}{\partial\theta} + \frac{1}{\sin\theta}\boldsymbol{e}_\phi\frac{\partial f}{\partial\phi} \tag{21}$$

$$\nabla_R = \boldsymbol{q} \times \frac{\partial f}{\partial \boldsymbol{q}} = \boldsymbol{e}_\phi\frac{\partial f}{\partial\theta} - \frac{1}{\sin\theta}\boldsymbol{e}_\theta\frac{\partial f}{\partial\phi} \tag{22}$$

Also, the operators are usually used with its derivatives:

$$\frac{\partial}{\partial \boldsymbol{q}}\boldsymbol{q} = \boldsymbol{I} - \boldsymbol{q}\boldsymbol{q} \tag{23}$$

$$\boldsymbol{q}\cdot\frac{\partial}{\partial \boldsymbol{q}} = \frac{\partial}{\partial \boldsymbol{q}}\cdot\boldsymbol{q} = 0,\ \frac{\partial}{\partial \boldsymbol{q}}\times\boldsymbol{q} = 0 \tag{24}$$

$$\left(\boldsymbol{q}\times\frac{\partial}{\partial \boldsymbol{q}}\right)\times\boldsymbol{q} = -2\boldsymbol{q} \tag{25}$$

$$\boldsymbol{q}\times\left(\boldsymbol{q}\times\frac{\partial}{\partial \boldsymbol{q}}\right) = -\frac{\partial}{\partial \boldsymbol{q}} \tag{26}$$

$$\nabla_R\cdot\nabla_R = \frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{27}$$

With these notations, the orientation is analyzed in the spherical coordinate system $\boldsymbol{q} = (\theta,\phi)$, with $\theta\in[0,\pi], \phi\in[0,2\pi)$. The $\theta = 0$ axis is chosen such that $\boldsymbol{q}\cdot\hat{\boldsymbol{H}} = \cos\theta$. The orientational distribution of $\boldsymbol{q}$ obeys the Boltzmann distribution, regardless of the translational location $\boldsymbol{x}$ of the swimmer:

$$P_0^\infty(d\Omega(\theta,\phi)) \propto \exp\left(-V(\boldsymbol{q})/k_BT\right)d\Omega, \tag{28}$$

where $d\Omega$ is the solid angle. The equilibrium distribution is:

$$P_0^\infty(\theta,\phi) = \frac{\sqrt{\chi_R}e^{\chi_R}}{2\pi^{3/2}\mathrm{Erfi}\left(\sqrt{\chi_R}\right)}\exp\left(-\chi_R\sin^2\theta\right), \tag{29}$$

and ϕ does not appear due to the axisymmetry. Here Erfi is the 'imaginary error function', and $\chi_R = \dfrac{\epsilon}{k_BT}$ is the dimensionless field strength. When $\chi_R = 0$, the orientational potential V vanishes and $P_0^\infty = 1/4\pi$.

Due to the symmetry of the field $V(\boldsymbol{q})$, the polar order, $\langle\boldsymbol{q}\rangle$, is zero, and the effect of the field is quantified by the nematic order parameter $\tilde{\boldsymbol{Q}} = \langle\boldsymbol{q}\boldsymbol{q}\rangle$, as shown in Fig. 1. When $\chi_R = 0$, $\tilde{Q}_\perp = \tilde{Q}_\parallel = 1/3$. When $\chi_R\to\infty$, all particles with the field $\boldsymbol{q} = \pm\hat{\boldsymbol{H}}$, and therefore $\tilde{Q}_\parallel = 1$ and $\tilde{Q}_\perp = 0$:

$$\left\langle\boldsymbol{q}_\parallel\boldsymbol{q}_\parallel\right\rangle = \frac{\exp(\chi_R)}{\sqrt{\pi}\sqrt{\chi_R}\mathrm{Erfi}\left(\sqrt{\chi_R}\right)} - \frac{1}{2\chi_R}, \tag{30a}$$

$$\left\langle\boldsymbol{q}_\perp\boldsymbol{q}_\perp\right\rangle = \frac{1}{2}\left(1 - \left\langle\boldsymbol{q}_\parallel\boldsymbol{q}_\parallel\right\rangle\right). \tag{30b}$$

Here by definition $\mathrm{Tr}\,\tilde{\boldsymbol{Q}} = 1$. The zero-traced nematic order parameter $\boldsymbol{Q} = \tilde{\boldsymbol{Q}} - \frac{1}{3}\boldsymbol{I}$, and $Q_\parallel = \left\langle\boldsymbol{q}_\parallel\boldsymbol{q}_\parallel\right\rangle - 1/3$, $Q_\perp = \left\langle\boldsymbol{q}_\perp\boldsymbol{q}_\perp\right\rangle - 1/3$.

The solution for $\boldsymbol{B}(\boldsymbol{q})$ is:

$$B_\parallel(\theta) = \int_0^{\cos\theta}\frac{1 - e^{\chi_R - \chi_R k^2}}{2\chi_R\left(k^2 - 1\right)}dk, \tag{31a}$$

$$B_\perp(\theta) = \cos\phi\sin\theta g(\cos\theta), \tag{31b}$$

where the function $g(x)$ in $B_\perp$ is the solution of the ODE:

$$\begin{aligned}&\left(x^2 - 1\right)g''(x) + 2x\left(\chi_R\left(x^2 - 1\right) + 2\right)g'(x)\\ &+ 2\left(\chi_R x^2 + 1\right)g(x) - 1 = 0.\end{aligned} \tag{32}$$

The function $g(x) = g(\cos\theta)$ satisfies (i) no singularities at $x = \cos\theta\to\pm1$, and (ii) is well-defined as $\chi_R\to0$. Thus,

$$\hat{D}_\parallel^{swim} = \frac{D_\parallel^{swim}}{U_0^2\tau_R/6} = 12\pi\int_0^\pi P_0^\infty\cos\theta\sin\theta\int_0^{\cos\theta}\frac{1 - e^{\chi_R - \chi_R k^2}}{2\chi_R\left(k^2 - 1\right)}dk\,d\theta, \tag{33a}$$

$$\hat{D}_\perp^{swim} = \frac{D_\perp^{swim}}{U_0^2\tau_R/6} = 6\int_0^{2\pi}\int_0^\pi P_0^\infty\sin^3\theta g(\cos\theta)\cos^2\phi\,d\theta\,d\phi, \tag{33b}$$

which are shown in Fig. 2.

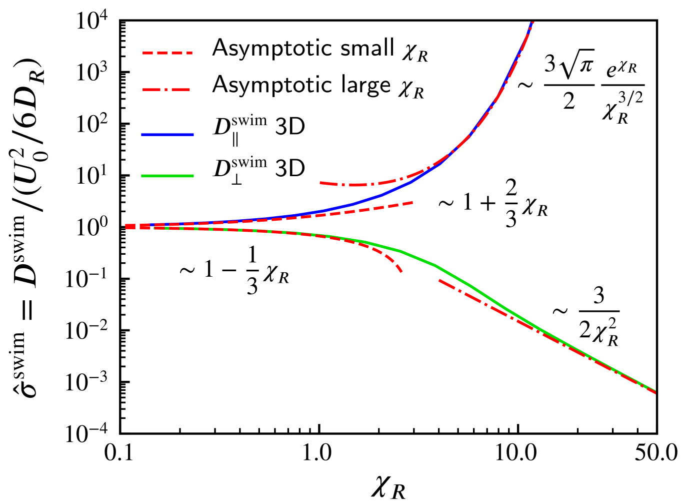

FIG. 2. The swim diffusivity $\boldsymbol{D}^{swim}$ in the directions parallel and perpendicular to the external field $\hat{\boldsymbol{H}}$ in 3D space. The solid lines are the analytical solutions (33).

From the swim diffusivity the swim stress follows as $\boldsymbol{\sigma}^{swim} = -n\zeta \boldsymbol{D}^{swim}$, and

$$\hat{\sigma}_{\parallel}^{swim} = \frac{\sigma_{\parallel}}{-n\zeta U_0^2/6} = \hat{D}_{\parallel}^{swim}, \tag{34}$$

$$\hat{\sigma}_{\perp}^{swim} = \frac{\sigma_{\perp}}{-n\zeta U_0^2/6} = \hat{D}_{\perp}^{swim}. \tag{35}$$

A. The weak-field limit $\chi_R \to 0$.

For weak fields a regular expansion of (33) gives:

$$\hat{\sigma}_{\parallel}^{swim} \approx 1 + \frac{2\chi_R}{3} + O(\chi_R^2), \tag{36a}$$

$$\hat{\sigma}_{\perp}^{swim} \approx 1 - \frac{\chi_R}{3} + O(\chi_R^2). \tag{36b}$$

As was the case for polar order aligned with $\hat{\boldsymbol{H}}$ induced by a potential with a single position of minimum energy [3], the swim pressure is decreased in the $\hat{\boldsymbol{H}}_{\perp}$ direction, because the energy barrier decreases the fluctuation of orientation $\boldsymbol{q}$ in that direction. The difference here, however, is that the stress in the $\hat{\boldsymbol{H}}$ direction is enhanced by the field. This is due to the bistable structure of the orientation potential, and we shall see a more significant effect in the strong-field limit.

B. The strong-field limit $\chi_R \to \infty$.

In this case, the swimmers may all align with either $\hat{\boldsymbol{H}}$ or $-\hat{\boldsymbol{H}}$, and only occasionally 'jump' between these two states. This is analogous to the famous Kramers' escape process [5], where a Brownian particle may jump out of a potential well slowly due to diffusion. As $\boldsymbol{q}$ is diffusive in rotation space, the jumping probability is modified from Kramers' original 1D estimation. The average jump time τ_j between the two directions is estimated to be [6]:

$$\tau_j = \frac{\sqrt{\pi}\exp(\chi_R)}{2\chi_R^{3/2}}\tau_R. \tag{37}$$

Physically, the swimmer may move in a direction with U_0 for τ_j and then jump to the other direction and move again with U_0 for another τ_j. Therefore, at times long compared to τ_R *and* τ_j, the diffusivity is simply a 1D random walk in the direction of $\hat{\boldsymbol{H}}$:

$$\hat{\sigma}_{\parallel}^{swim} = \frac{D_{\parallel}^{swim}}{U_0^2\tau_R/6} \to \frac{3\sqrt{\pi}\exp(\chi_R)}{2\chi_R^{3/2}}. \tag{38}$$

It is important to note that one must wait a time long compared to τ_j before the limiting behavior is obtained and this time grows exponentially with the field strength χ_R.

In addition to moving in the $\pm\hat{\boldsymbol{H}}$ directions, the swimmers also move in the direction perpendicular to $\hat{\boldsymbol{H}}$, due to small fluctuations around $\pm\hat{\boldsymbol{H}}$ driven by D_R. Following this route, the distribution of the fluctuation field $B_\perp$ can be approximated with a singular 'boundary layer' around the parallel direction. After the tedious mathematics is properly handled, the result is very simple:

$$\hat{\sigma}_{\perp}^{swim} = \frac{D_{\perp}^{swim}}{U_0^2\tau_R/6} \to \frac{3}{2\chi_R^2}, \tag{39}$$

as $\chi_R \to \infty$. The asymptotic predictions are shown in Fig. 2 and are in excellent agreement with the full solutions.

IV. THE POLAR ORDER IN THE BOUNDARY LAYER

From the microscopic colloid perspective, the swimmers form a kinetic boundary layer [7] on the wall with directed motion as shown in Fig. 3. More specifically, on a microscopic scale close to the wall, there is net polar order $\boldsymbol{m} = \int P\boldsymbol{q}d\boldsymbol{q} \neq 0$, even though the nematic orientation field has no polar order in the bulk. This boundary layer structure for two cases $\chi_R = 0.4$ and $\chi_R = 1.6$ are shown in Fig. 3, with the FEM solution to the probability density $P(z,\theta)$.

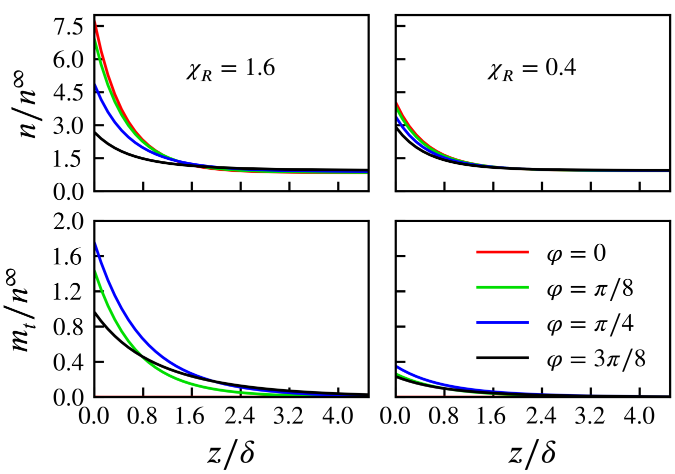

FIG. 3. The boundary-layer structure for the case of $\chi_R = 1.6$ (left column) and $\chi_R = 0.4$ (right column), taken from the same data as shown in Fig. 4 of the main text. Here n^∞ is the number density in the bulk, corresponding to the n in Fig. 3 and Fig. 4 of the main text. The boundary-layer thickness z is scaled with the microscopic length $\delta = \sqrt{D_T\tau_R}$. The tangential component of polar order $m_t = \boldsymbol{m}\cdot\boldsymbol{t}$. For the $\hat{\boldsymbol{H}}$ in Fig. 1 of the main text, m_t is towards the left on the bottom wall. For $\varphi = 0$, $m_t = 0$ everywhere..

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